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COMPUTER STUDIES OF SHOCK-INDUCED PROCESSES*

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SUMMARY

The study of shock propagation and shock-induced processes in condensed matter is a rapidly-expanding interdisciplinary area involving engineering, chemistry, and physics to which the application of computer molecular dynamics has begun to make valuable contributions. In addition to the ever-increasing interest in the properties of shock disturbances in condensed media, there is a growing awareness of the importance of understanding the microscopic details underlying shock-induced chemical processes and phase transformations. An important specific example is to be found in the study of energetic, or explosive, materials where an understanding of the shock-initiation process (i.e., how shock loading begins the first steps in the chemistry of dissociation and subsequent bond reformation) can be of great practical importance. If the initial and transitional stages of the processes involved (both the chemistry and physics) are understood, the probability for affecting those same processes is thereby enhanced.

We have completed, over the past three years, a large number of molecular dynamics calculations of the effects of the interaction of shock waves in condensed systems. We have explored the microscopic effects of material characteristics known to cause changes in the sensitivity of explosives -- voids and cracks, crystal defects, inclusions, initial temperature, and shock strength, and we have found a very instructive correlation with the macroscopic results. We have found that the role played by imperfections and irregularities in providing channels for coupling the energy localized in the

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shock front to the lattice modes is quite significant, particularly when these imperfections are located near one of the surfaces. The general disruption of the lattice that occurs in the vicinity of all types of imperfections and from the spalling of surface material gives birth to energetic atomic and molecular fragments that can certainly be expected to play an important role in the ensuing chemical reactions.

During the presentation the influence of structural discontinuities such as voids, grain boundaries, and other point and line defects, and of the free surface on dissociation will be emphasized. A film summary of these calculations will be presented.

FIGURE CAPTIONS

Figure 1. Reaction zone macrodynamics. Upper curves are pressure in GPa and percent of high explosive that has reacted as a function of time or distance in a detonation. Lower curves are similar information for a weak initiation.

Figure 2. Shock loading in one-dimensional and two-dimensional model lattice systems. The analytical impulsive force F(t) versus time t is shown. A typical displacement profile U_n and velocity profile V_n are also shown, where n indexes the atoms along the chain (or lattice columns in the two-dimensional lattice).

Figure 3. Representative interactomic potentials for Morse (inert), reactive, and metastable lattices.

Figure 4. Plate impact on a lattice with the subsequent spall.

Figure 5. Shock transit through a three-dimensional lattice showing the microscopic spall that occurs when the shock front meets a free surface.

Figure 6. Shock interactions with voids, point defects, free surfaces, and line defects.

Figure 7. Initial configuration for all impact-loaded void studies considered.

Figure 8. The impact-loaded model void at finite temperatures: (a) a shock launched in the first wall, (b) spall commencing from the inner face of the first wall, (c) the fragment spalled from the first wall transiting the void, (d) the spalled fragment striking the inner face of the second wall, (e) spall beginning to form from the outer face of the second wall, and (f) a much later stage. Initially the lattice is at room temperature.

Figure 9. The impact-loaded metastable lattice: (a) the initial state, (b) immediately following impact, (c) shock transiting the lattice, (d) shock transit terminating as it reaches the far end, (e) spall developing from the surface, and (f) a later stage showing well-developed spall behind which a lattice with a different crystalline structure has formed. Disintegration of the lattice is occurring well to the rear because of energy released in the exothermic polymorphic transitions.

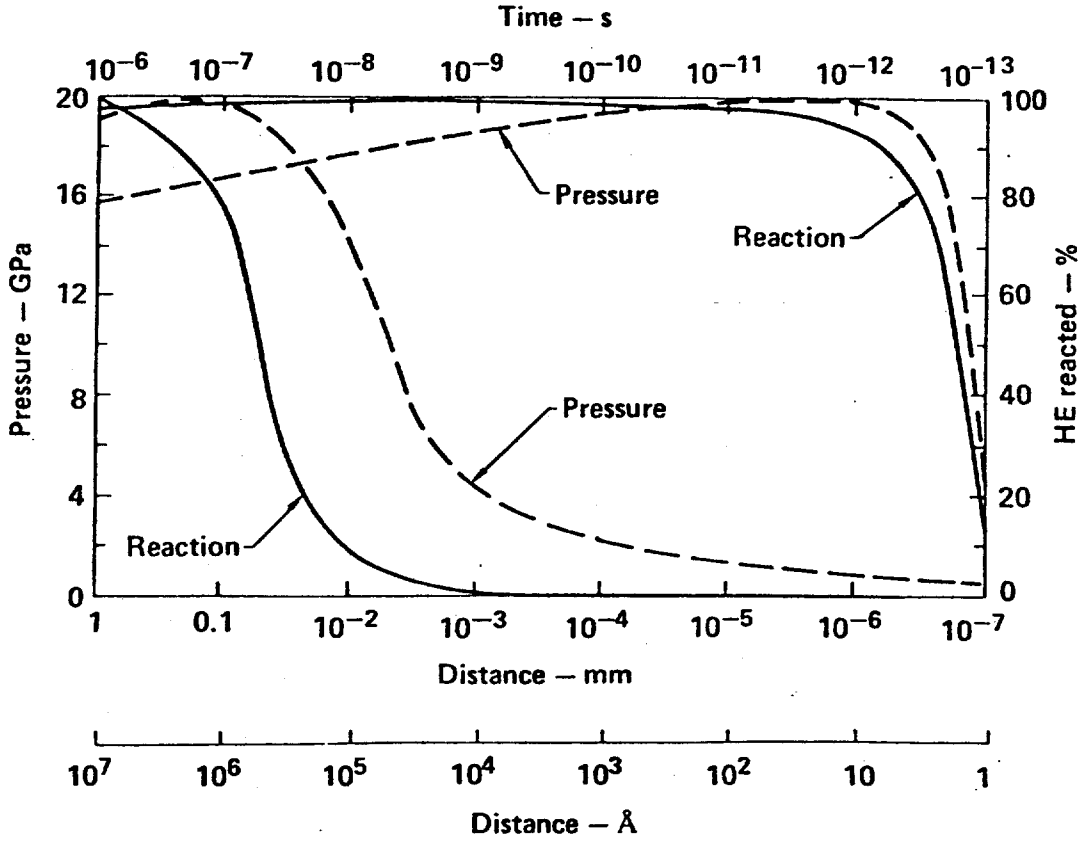

Time – s
10^-6 10^-7 10^-8 10^-9 10^-10 10^-11 10^-12 10^-13
Pressure – GPa
HE reacted – %
20 16 12 8 4 0
100 80 60 40 20 0
Pressure
Reaction
Pressure
Reaction
1 0.1 10^-2 10^-3 10^-4 10^-5 10^-6 10^-7
Distance – mm
10^7 10^6 10^5 10^4 10^3 10^2 10 1
Distance – Å

Figure 1.

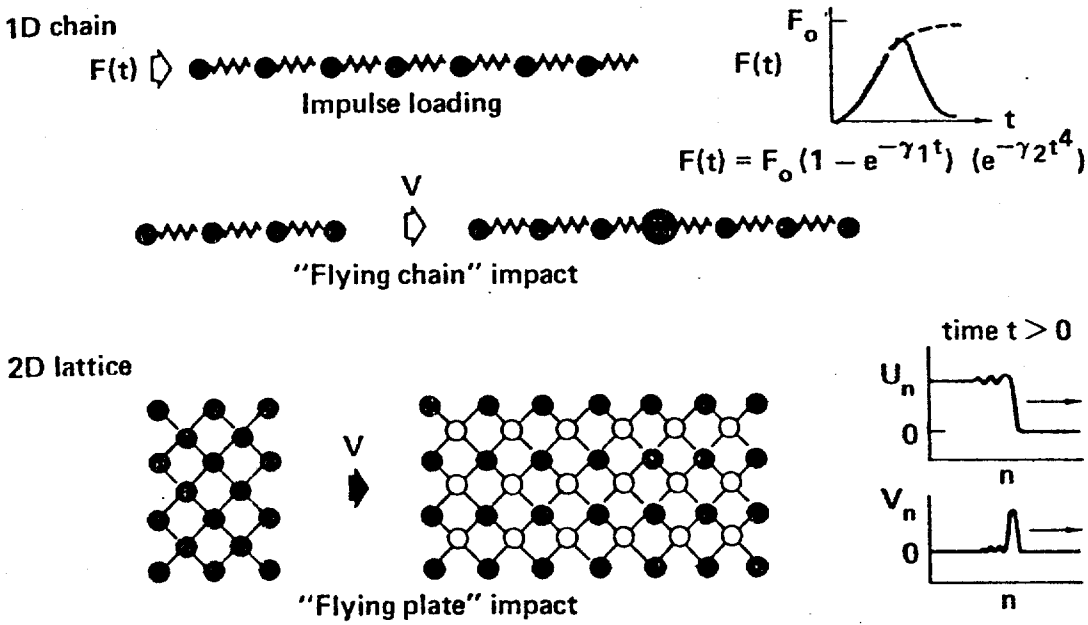
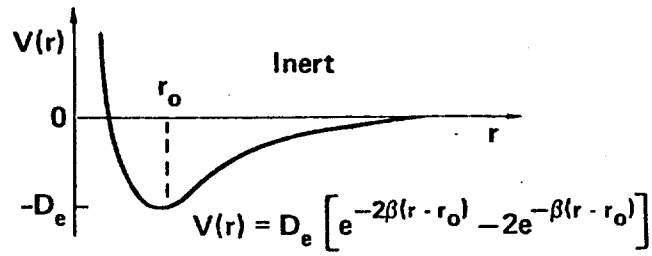

1D chain
F(t)
Impulse loading
F_o
F(t)
t
$F(t) = F_o(1 - e^{-\gamma_1 t})\ (e^{-\gamma_2 t^4})$
V
"Flying chain" impact
2D lattice
V
"Flying plate" impact
time t > 0
U_n
0
n
V_n
0
n

Figure 2.


V(r)
Inert
r_o
0
r
$-D_e$
$V(r) = D_e \left[e^{-2\beta(r - r_o)} - 2e^{-\beta(r - r_o)} \right]$

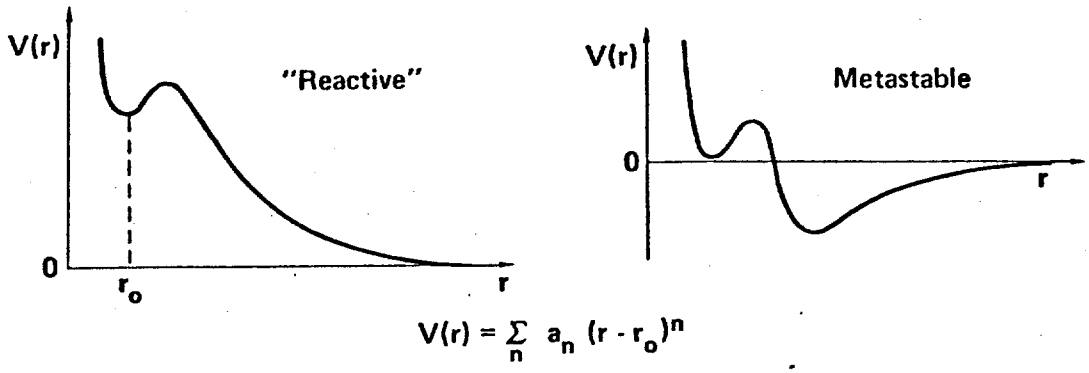

V(r)
"Reactive"
0
r_o
r
V(r)
Metastable
0
r
$V(r) = \sum_n a_n (r - r_o)^n$

Figure 3.

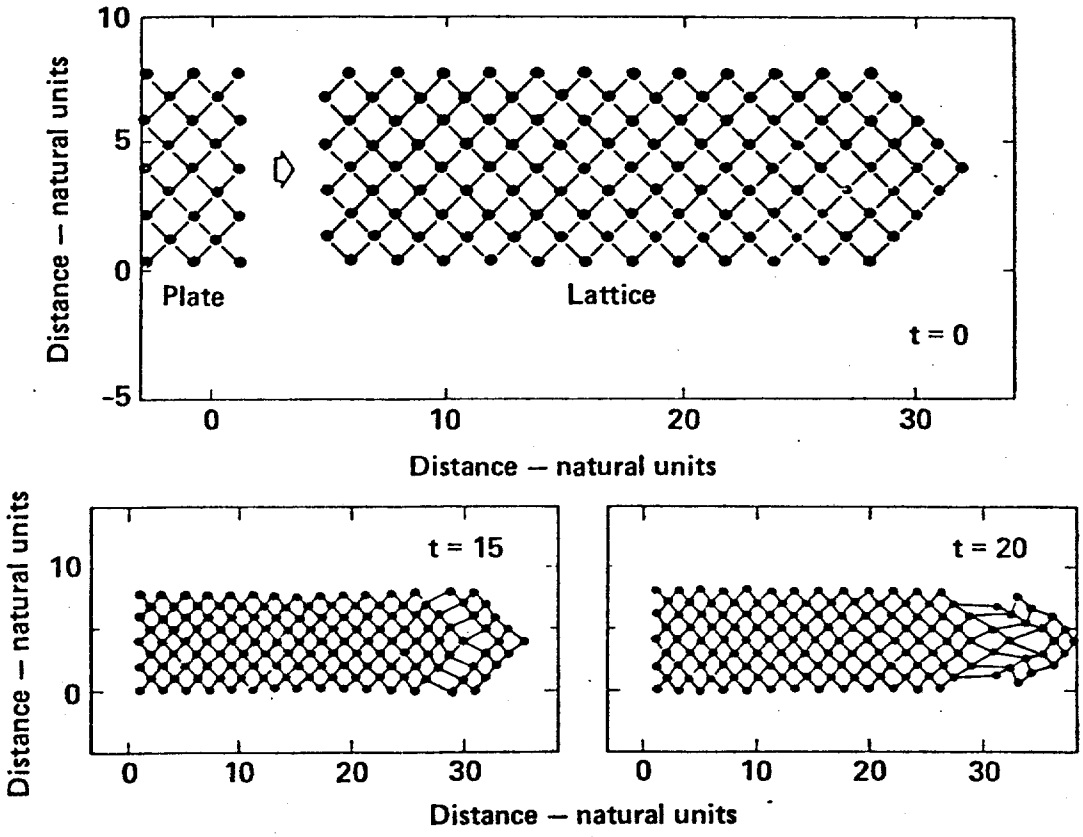

10
5
0
-5
Distance — natural units
Plate
Lattice
t = 0
0
10
20
30
Distance — natural units
t = 15
t = 20
Distance — natural units

Figure 4.

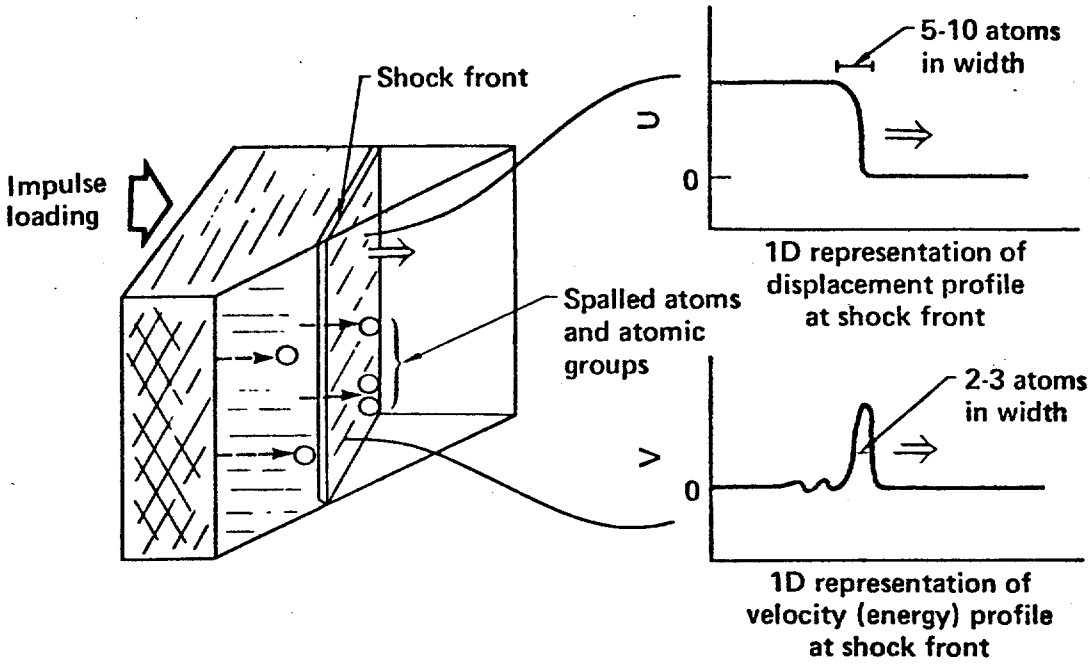
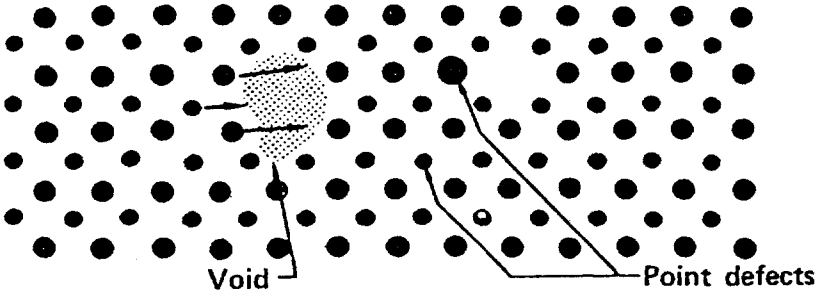
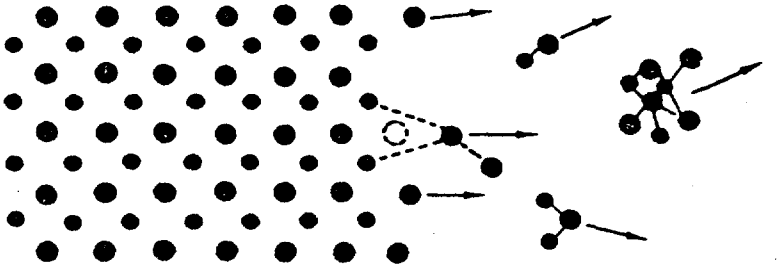

Impulse loading
Shock front
Spalled atoms and atomic groups
5-10 atoms in width
0
1D representation of displacement profile at shock front
2-3 atoms in width
0
1D representation of velocity (energy) profile at shock front

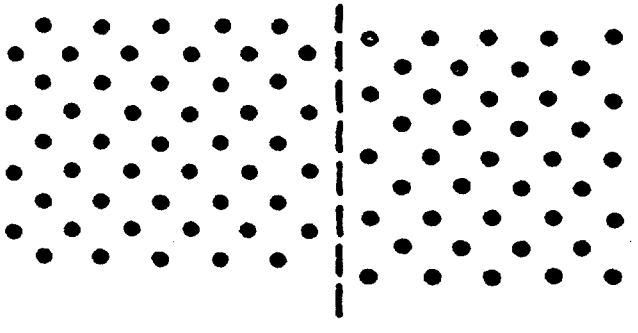
Figure 5.



Voids and point defects



Spalling of atoms and atomic fragments



Line defects and grain boundaries

Figure 6.

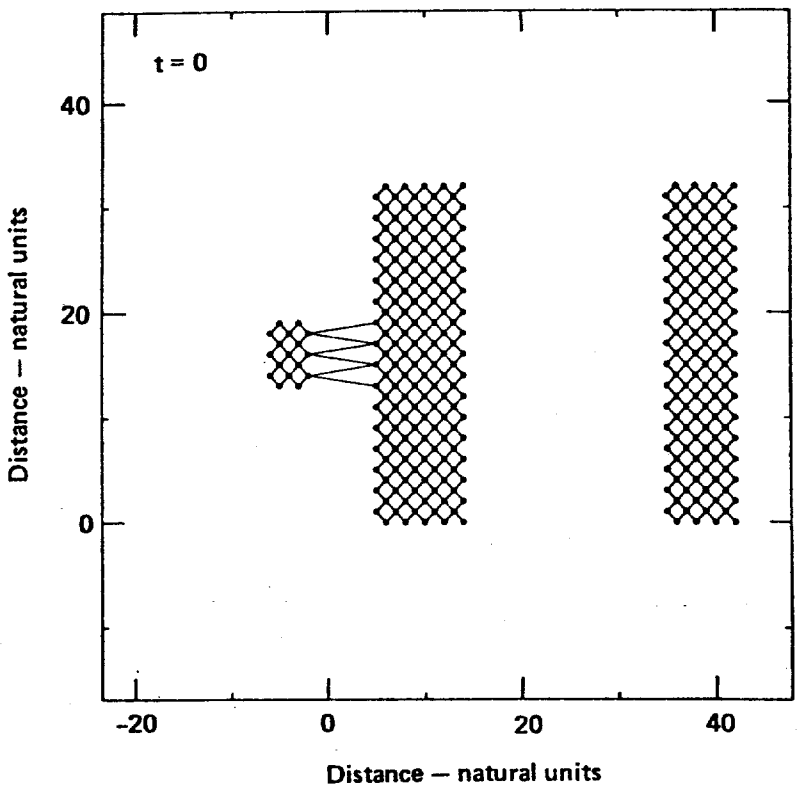

t = 0
40
20
0
-20
0
20
40
Distance — natural units
Distance — natural units

Figure 7.

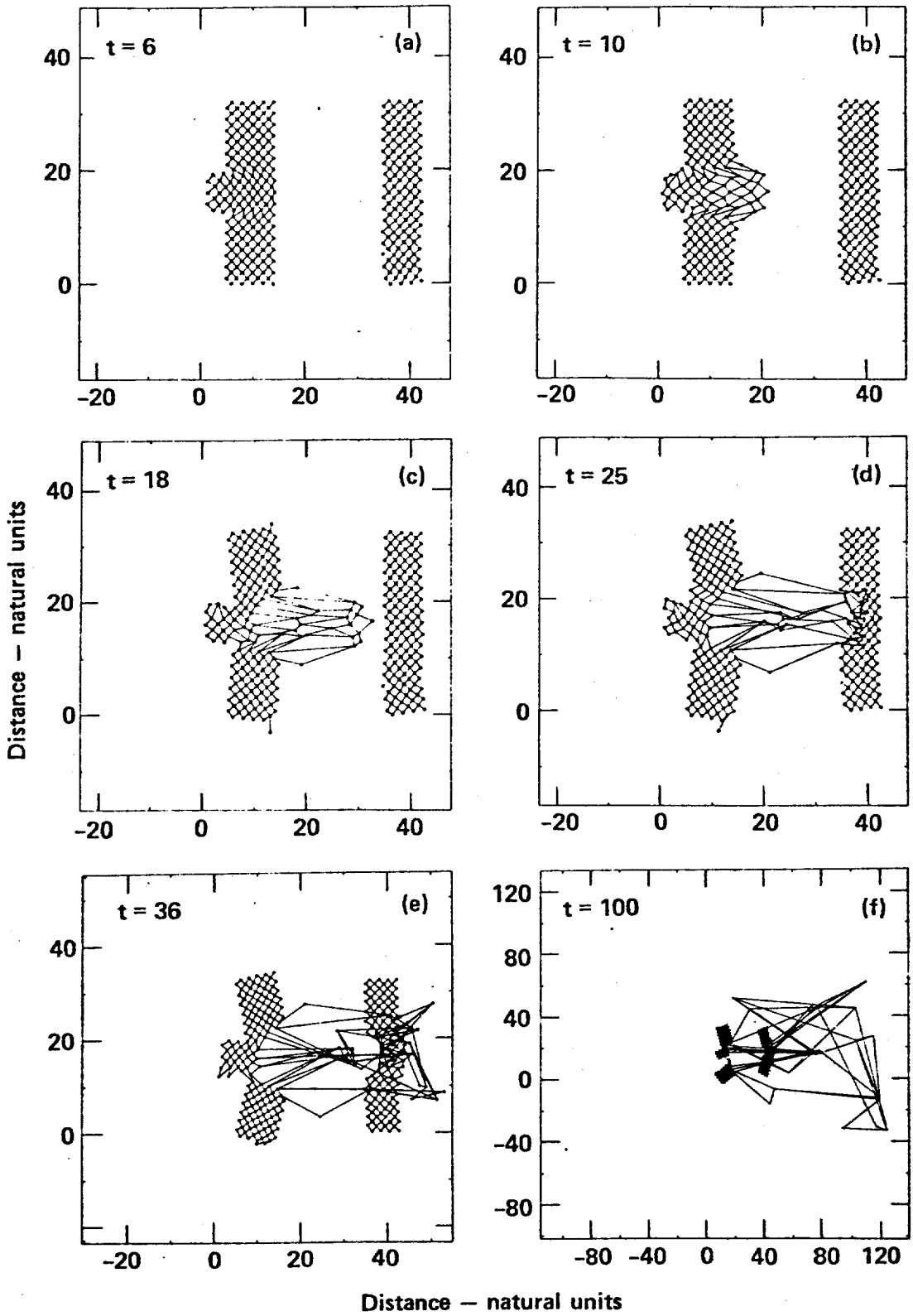

t = 6
(a)
t = 10
(b)
t = 18
(c)
t = 25
(d)
t = 36
(e)
t = 100
(f)
Distance — natural units
Distance — natural units

Figure 8.

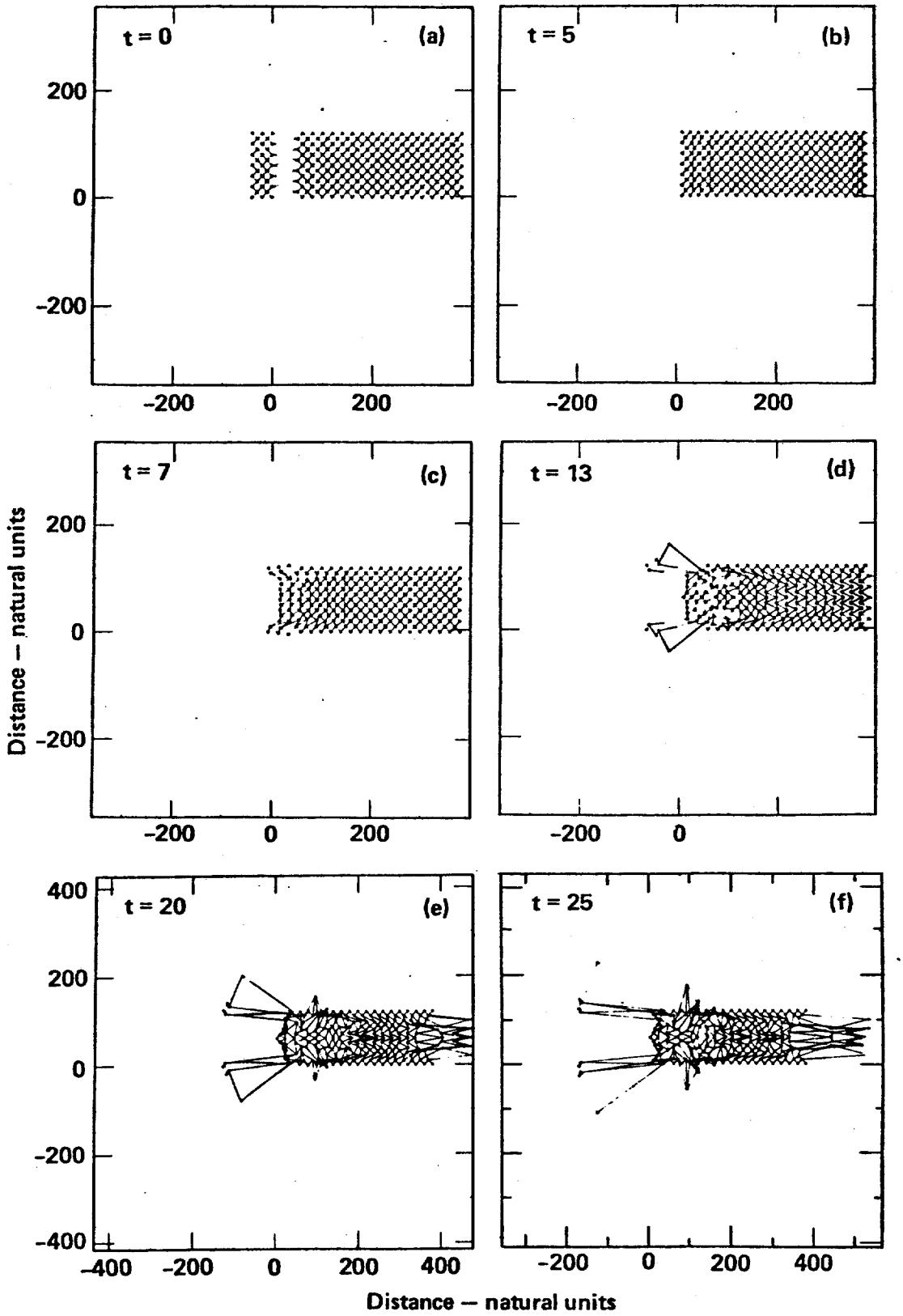

t = 0
(a)
t = 5
(b)
t = 7
(c)
t = 13
(d)
t = 20
(e)
t = 25
(f)
200
0
-200
400
-400
Distance — natural units
Distance — natural units

Figure 9.

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